Interaction of the Torque-Induced Elastic Charge and Elastic Dipole with a Wall in a Nematic Liquid Crystal.

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(Dated: February 23, 2009)

Abstract

We show that the elastic charge of colloids in a nematic liquid crystal can be generated by the vector of external torque. The torque components play the role of two component charge (dyad) and give rise to the Coulomb-like potential, while their conservation law plays the role similar to that of Gauss' theorem in the electrostatics. The theory is applied to the colloid-surface interaction. A wall with homeotropic or planar director is shown to induce a repulsive $1/r^4$ force on the elastic dipole. The external torque, however, induces the elastic charge in this colloid and triggers switching to the $1/r^2$ repulsion.

Keywords: nematic emulsion, elastic charge, colloid-wall interaction.

Short title: elastic charge-wall interaction.

I. INTRODUCTION

Particles of a submicron and micron size immersed in a nematic liquid crystal (NLC) interact via the director field $\mathbf{n}$ which mediates the distortions induced by their surfaces [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. The new field of nematic colloidal systems, or nematic emulsions [10], has gained a continuous growing interest over the past few years. The physics of these anisotropic colloidal systems has a deep similarity to the electrostatics. It has been shown that the director-mediated interaction is of a long range and possesses many other properties characteristic of the interaction between electric dipoles and quadrupoles [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. Particle trapping techniques [12] have been used to test this analogy and demonstrate experimentally the dipole-dipole [13, 14], quadrupole-quadrupole [15, 16], and mixed disclination-dipole [17] pair interactions. Reorientation of the elastic dipoles was shown to be responsible for phase transitions between different 2-dimensional colloidal lattices on a nematic-air interface [18]. In the context of this analogy it is natural to expect that the Coulomb interaction, which is fundamental to the electrostatics, has an important implication in the physics of nematic emulsions, too. Recently we developed the electrostatic analogy in nematic emulsions to the level of charge and its density [19, 20]. The director-mediated Coulomb-like interaction of two colloids was shown to be fully determined by vectors $\mathbf{\Gamma}_\perp^{(1)}$ and $\mathbf{\Gamma}_\perp^{(2)}$ of the transverse external torques (perpendicular to the unperturbed director at infinity) applied on the colloids [19, 20]. The scalar product $-(\mathbf{\Gamma}_\perp^{(1)} \cdot \mathbf{\Gamma}_\perp^{(2)})$ plays the role of the product of two electrostatic charges in the $1/r$ interaction potential, and thus the two components of external torque play the role of two component elastic charge. Because of the difference between the scalar electrostatics and vector nematostatics, the elastic analogues of the surface charge density, charge, and higher multipole moments consist of two tensors (dyad). The multipole moments are naturally expressed via the elastic charge density which is determined by the two transverse director components on the surface imposing the director deformations. The interaction of the axially-symmetric sources, considered phenomenologically in [7], obtains as particular case of the interaction of two correspondent multipole dyads. Small parameter of the theory is the ratio $a/r =$ (colloid size/distance between colloids). For small a/r the theory provides all the tools available in the electrostatics, e.g., for solving different boundary problems that can occur in the nematostatics of anisotropic emulsions. In this paper we apply the nematostatics developed

in [19, 20] to the interaction between an elastic charge (dyad) and elastic dipole (dyad) with a wall (surface bounding the NLC) with different director alignments, which is the elastic counterpart of the well-known electrostatic problem solved by the method of images. In the next section we briefly introduce the colloidal nematostatics of Ref.[19, 20] and show that the integral form of the torque balance plays the role similar to that of Gauss' theorem in the electrostatics. Then the theory is applied to the colloid-surface interaction. A wall with homeotropic or planar director is shown to induce a repulsive $1/r^4$ force on the elastic dipole. The external torque, however, induces the elastic charge in this colloid and triggers switching to the $1/r^2$ repulsion. These results suggest that predictions of the colloidal nematosctatics can be tested by observing behavior of a single colloid at a sample surface which, in some situations, can be more robust than dealing with two colloids.

II. ELASTIC CHARGE DENSITY REPRESENTATION OF THE COLLOIDAL NEMATOSTATICS

A. Torque balance, Gauss' theorem, and elastic charge in 3 dimensions.

The fundamental physical quantity of electric charge is purely phenomenological and must be *postulated* in the theory of elementary particles. In contrast, the nematostatics of the director field **n** allows for *introduction* of two different charges. Electrostatic potential is a scalar described by the linear Laplace (or Poisson) equation. It is the linearity that underlies the definition of the electric charge and its density as the source of electric field. At the same time, **n** is a vector field which reduces to a single variable, described by a linear equation (in the one constant approximation), only in 2 dimensions (2d). Owing to the linearity, the deformation source can be straightforwardly established: core of a point defect plays the role of a charge in 2d [21, 22, 23, 24]. The independence of the integral, expressing the topological invariant, of the integration contour plays the role anlogous to Gauss' theorem in electrostatics, the invariant itself plays the role of a conserved charge, and the 2d nematostatics is similar to the 2d electrostatics with its logarithmic potential: disclinations of the same signs repel and those of the opposite signs attract each other.

In 3d, however, the analogy between topological defects and charge is completely lost. In 3d, the field **n** is described by highly nonlinear equations [21] so that point defects, though

remain topological invariants, cannot be linearly connected with the distortions of $\mathbf{n}$ they induce [7, 10]. Here the deformation sourse is the director distribution around the particle in its close vicinity of a size $\sim a$. We refer to such the deformation domain as particle though the distortion therein can be induced by surface of a real particle, by topological defects with zero total topological charge [7, 10], or by an external field dying out outside the domain area, Fig. 1. Consider 3-d director field $\mathbf{n}(\mathbf{r})$, uniform and parallel to the z-axis at infinity, $\mathbf{n}_\infty = (0, 0, 1)$. At distances $r \gg a$, the small particle-induced perturbation n_t of $\mathbf{n}_\infty$ is transverse, $t = x, y$, and (in the one-constant approximations assumed in this paper) has the form

$$n_t(\mathbf{r}) = \frac{q_t}{r} + 3\frac{(\mathbf{d}_t \cdot \mathbf{r})}{r^3} + 5\frac{(\mathbf{Q}_t : \mathbf{r} : \mathbf{r})}{r^5} + ..., \tag{1}$$

It is natural to identify the coefficients with the subscript t in this expansion with the t-th component of elastic charge, elastic dipole, and elastic quadrupole, respectively. We seek the elastic analog of charge, following de Gennes' idea outlined in [21]. A transverse external torque $\mathbf{\Gamma}_\perp = (\Gamma_x, \Gamma_y, 0)$ applied on a particle in the equilibrium is balanced by another, the elastic torque distributed over a surface S enclosing the particle, i.e.,

$$\Gamma_t = K \int_S \varepsilon_{\alpha t \rho}(r_\rho \partial_\beta n_\gamma \partial_\alpha n_\gamma + n_\rho \partial_\beta n_\alpha) dS_\beta, \tag{2}$$

whrere K is the elastic constant, $\varepsilon_{\alpha t \rho}$ is the absolute antisymmetric tensor, all indices but t run over $1, 2, 3$, and summation over the repeated indices is implied. The integral in the r.h.s. does not depend on the choice of enclosing surface S, and the equality (2) reminds one Gauss' theorem with Γ_t in place of the electric charge. To further justify this connection one notices that integral (2) over a remote surface S vanishes for any term in the expansion (1) but the first one. Substituting $n_t = q_t/r$ in (2) and integrating over a large sphere gives $\Gamma_y = 4\pi K q_x$, $\Gamma_x = -4\pi K q_y$, or

$$q_t = \frac{[\mathbf{\Gamma} \times \mathbf{n}_\infty]_t}{4\pi K}. \tag{3}$$

Thus, the tentative conclusion is that, in 3d, the role of Gauss' theorem and charge is played, respectively, by the balance of external and elastic torques (conservation of torque) and by the transverse components of the external torque exerted on the particle. This

is fully justified by calculating the Coulomb-like interaction in the elastic charge density representation developed in [19, 20].

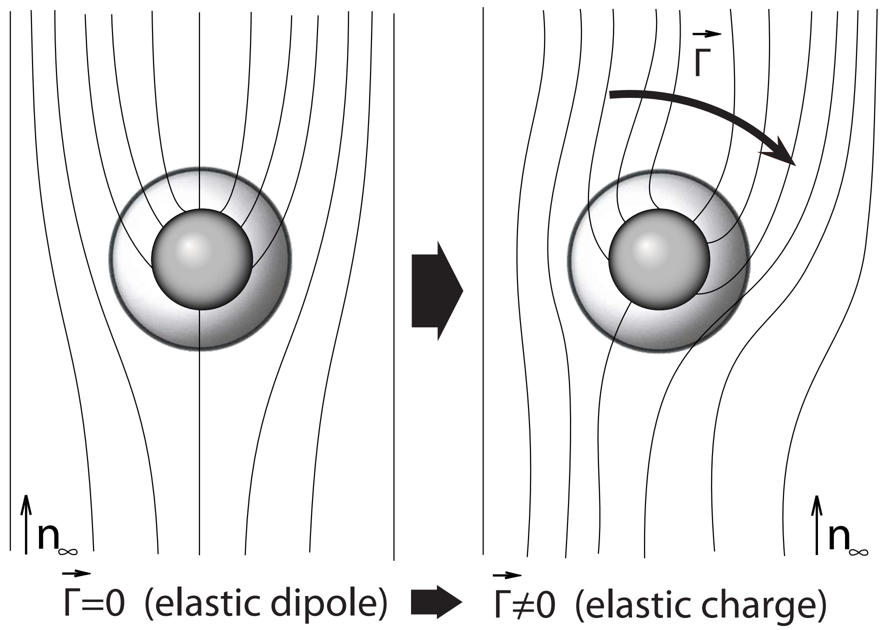

FIG. 1: General deformation source ("partcile') in 3d. Inside the gray sphere the deformations can be very large (e.g., induced by point defects or strong anchoring of a real colloid). But outside the larger sphere the deformations are weak and linear which allows for the electrostatic anlogy. The particle itself is of the dipolar type, but an external torque upon it can charge it, and it becomes an elastic charge.

B. Dyads of elastic mutipoles and their interaction via the director field: the outline

The results of Refs. [19, 20] instructive to our task here can be summarized as follows. Consider a deformation source with the director distributions n_t given on the surface of enclosing sphere S with radius a. The quantity

$$\sigma_t(\mathbf{s}) = n_t(\mathbf{s})/a^2, \tag{4}$$

plays the role of two component surface elastic charge density on the sphere S. Using natural analogy with the electrostatics, we define the two component elastic multipoles via the surface charge density as the following integrals over sphere S enclosing the particle:

$$q_t = \frac{a}{4\pi}\int_S \sigma_t d^2 s, \tag{5}$$

$$d_{t,\alpha} = \frac{a^2}{4\pi}\int_S \sigma_t \nu_\alpha d^2 s, \tag{6}$$

$$Q_{t,a\beta} = \frac{a^3}{8\pi}\int_S \sigma_t (3\nu_\alpha \nu_\beta - \delta_{\alpha\beta}) d^2 s, \tag{7}$$

where ν is the vector of a unit outer normal to S. With these definitions, we obtained the interaction of two particles with similar multipoles. Interaction of two "charged" particles with nonzero q_t is Coulomb-like:

$$U_{Coulomb} = -4\pi K \frac{q_t^{(1)} \cdot q_t^{(2)}}{R} = -\frac{(\mathbf{\Gamma}_\perp^{(1)} \cdot \mathbf{\Gamma}_\perp^{(2)})}{4\pi K R}, \tag{8}$$

where we used relation (3), $\mathbf{\Gamma}_\perp^{(i)} = \mathbf{\Gamma}^{(i)} - (\mathbf{\Gamma}^{(i)} \cdot \mathbf{n}_\infty)$ is the transverse component of the torques exerted upon the i-th particles, and R is the modulus of the separation vector $\mathbf{R}$. The above connection between the elastic charge and external torque is thus fully justified. Eq. (8) shows that, depending on the sign of $(\mathbf{\Gamma}_\perp^{(1)} \cdot \mathbf{\Gamma}_\perp^{(2)})$, the elastic Coulomb interaction can be attractive or repulsive. In contrast to the electrostatics and 2d nematostatics, the charges with the same sign attract and with different signs repel each other ("parallel torques" attract whereas two "antiparallel torques" repel each other). Although the colloids must be anchored to the director, the Coulomb-like interaction does not directly depend on their specific shape and anchoring. Instead, the elastic charge is determined by the coefficients describing the torque exerted upon the colloid by a given type of external field. For instance, this can be the vector of permanent electric and magnetic dipole or electric and magnetic polarizability tensors of a given colloid.

If the external torques are absent, the interaction energy is expressed solely in terms of particles' multipoles. The interaction between two "dipolar" particles is of the form

$$U_{dd} = -12\pi K \frac{(\mathbf{d}_t^{(1)} \cdot \mathbf{d}_t^{(2)}) - 3(\mathbf{d}_t^{(1)} \cdot \mathbf{u})(\mathbf{d}_t^{(2)} \cdot \mathbf{u})}{R^3}, \tag{9}$$

where $\mathbf{u} = \mathbf{R}/R$ is a unit vector along the separation direction. Eqs.(1),(4)-(9) (along with the quadrupole-quadrupole potential derived in [19, 20]) suggest the following interpretation. q_t is the t-th component of the elastic charge and $\sigma_t(\mathbf{s})$ is its surface density at point $\mathbf{s}$ on the sphere. The vector $\mathbf{d}_t$ and tensor $\mathbf{Q}_t$ are the t-th dipole and quadrupole moments

determined in the standard way by the surface charge density σ_t on the sphere. As σ_x and σ_y are separate sources, they determine not only the x and y director components outside the particle, Eq.(1), but also two independent tensors (dyad) for each multipole moment, i.e., q_x and q_y, $\mathbf{d}_x$ and $\mathbf{d}_y$, $\mathbf{Q}_x$ and $\mathbf{Q}_y$, and so on.

III. COLLOID-WALL INTERACTION IN A NEMATIC LIQUID CRYSTAL

The above formulas can be used to solve boundary problems similar to those of electrostatics. The simplest boundary problem is the interaction of an elastic multipole with a surface bounding the nematic sample and imposing planar or homeotropic director alignment. Here we consider this problem for an elastic charge and dipole.

A. Repulsion of an elastic charge from the wall

Let us consider a single particle with a charge at a distance h from a plane surface of a NLC sample. We assume that the anchoring is strong, the director alignment in the sample $\mathbf{n}_\infty$ far from the particle is homogeneous and parallel to the z-axis, $\mathbf{n}_\infty = (0, 0, 1)$,but the angle it makes to the surfaces is arbitrary. The charge q_t can be induced by an external field exerting the torque $\mathbf{\Gamma}$ with the components $\Gamma_y = 4\pi K q_x$ and $\Gamma_x = -4\pi K q_y$. To justify the linearized theory, h is assumed to be large compared to the particle' size. As the director on the sample surface is fixed, the boundary condition is $\mathbf{n}_t = 0$, $t = x, y$.

The problem can be solved using the mirror-image method. Let us place the image-particle with the charge $q_t^{'}$ on the other side of a surface at distance h from it, Figs.2,3. For large h, distortions induced by the charge and its image are given by the sum (see Eq.(1)):

$$n_t(\mathbf{r}) = \frac{q_t}{r_1} + \frac{q_t^{'}}{r_2}, \tag{10}$$

where r_1 and r_2 are the distances from a given point of the wall to the location of the charge and its image. As $r_1 = r_2$, the boundary condition is satisfied for $q_t = -q_t'$, $t = x, y$. The fact that the particle and its image are oppositely charged means that $\mathbf{\Gamma}_\perp = -\mathbf{\Gamma}_\perp^{'}$, Figs.2,3. As two opposite elastic charges repel each other, the elastic charge-wall interaction is repulsive. The repulsion force obtains from the interaction energy (8) of the torques $\mathbf{\Gamma}_\perp$ and $-\mathbf{\Gamma}_\perp$ by differentiating with respect to R at $R = 2h$, i.e.,

$$F_q = \frac{\mathbf{\Gamma}_\perp^2}{16\pi K h^2}. \tag{11}$$

The result depends on the direction of $\mathbf{n}_\infty$ and thus on the surface tilt via the relation $\mathbf{\Gamma}_\perp = \mathbf{\Gamma} - (\mathbf{\Gamma} \cdot \mathbf{n}_\infty)$.

B. Repulsion of an elastic dipole from the wall

Now consider the interaction between a wall and an elastic dipole represented by dyad $(\mathbf{d}_x, \mathbf{d}_y)$, Eq.(6). In general, each of the two vectors $\mathbf{d}_x$ and $\mathbf{d}_y$ has three nonzero components. Symmetry makes some of them vanish. For ellipsoids with one of their axes along $\mathbf{n}_\infty = (0,0,1)$, the dipole dyad is diagonal: $\mathbf{d}_x = (d_x, 0, 0)$, $\mathbf{d}_y = (0, d_y, 0)$ where $d_x \neq d_y$. In the case of an axially symmetric particle with symmetry planes passing through the symmetry axis assumed to be along $\mathbf{n}_\infty$, $d_x = d_y = d$ (note that an axially symmetric particle without symmetry planes, such as a helicoid, is a chiral source which will be considered elsewhere). We restrict our consideration to this simple and practically important case of colloids. For instance, such are the so-called "topological dipoles", i.e., spherical particles with homeotropic boundary conditions with a companion hyperbolic hedgehog or disclination ring [7, 10].

From the general equation (9), the interaction energy of two axially symmetric dipolar particles with nonzero components $d^{(1)}$ and $d^{(2)}$ obtains in the form

$$U_{dd} = \frac{12\pi K d^{(1)} d^{(2)}}{R^3}(1 - 3\cos^2\theta), \tag{12}$$

where θ is the angle the separation vector $\mathbf{R}$, which, in our geometry, is along the surface normal, makes with the far homogeneous director $\mathbf{n}_\infty$. This formula, up to the coefficient 3, reproduces the one obtained for the axially symmetric "topological dipoles" in [7, 10].

Consider an elastic dipole dyad $\mathbf{d}_t$, $t = x, y$, at a distance h from the sample surface (wall). The z-direction is along the unperturbed homogeneous director $\mathbf{n}_\infty = (0,0,1)$.The general boundary condition on a surface with strong anchoring of any type is again $\mathbf{n}_t = 0$, $t = x, y$. The image-dipole $\mathbf{d}_t'$ is located at the distance h on the opposite side of the wall. The director field at point $\mathbf{r}$ of the surface is

$$n_t(\mathbf{r}) = 3\frac{(\mathbf{d}_t \cdot \mathbf{r}_1)}{r_1^3} + 3\frac{(\mathbf{d}_t^{'} \cdot \mathbf{r}_2)}{r_2'^3}, \tag{13}$$

where $\mathbf{r}_1 =$ and $\mathbf{r}_2$ are separation vectors between point $\mathbf{r}$ of the surface and the particle and its image. The boundary condition $\mathbf{n}_t = 0$ gives two equations, i.e.,

$$(\mathbf{d}_t \cdot \mathbf{r}_1) + (\mathbf{d}_t' \cdot \mathbf{r}_2) = 0,\ t = x, y. \tag{14}$$

We will consider the wall with the planar and homeotropic director alignment individually.

a. Planar wall. The wall with a planar director alignment, Fig.4, coincides with the yz-plane $x = 0$, while the x-axis is normal to the wall. Obviously, if $\mathbf{r}_1 = (-x, y, z)$, then $\mathbf{r}_2 = (x, y, z)$. The two equations (14) then are solved by $\mathbf{d}_x = \mathbf{d}_x^{'}$ and $\mathbf{d}_y = -\mathbf{d}_y^{'}$, Fig 4. The interaction energy of the dipole dyad $(\mathbf{d}_x, \mathbf{d}_y)$ and its image $(\mathbf{d}_x, -\mathbf{d}_y)$ is readily calculated from eq.(9) by substituting $\mathbf{d}_x = (d, 0, 0)$ and $\mathbf{d}_y = (0, d, 0)$. The force is obtained by differentiating this expression with respect to $\mathbf{R}$ at $R = 2h$. This gives a repulsive force with the magnitude

$$F_{d,planar} = 4\pi K \frac{27d^2}{32h^4}. \tag{15}$$

b. Homeotropic wall In the homeotropic geometry, Fig. 5, the uniform director and the z-axis with the onset at the wall are normal to the wall which coincides with the xy-plane. Obviously, if $\mathbf{r}_1 = (x, y, -z)$ then $\mathbf{r}_2 = (x, y, z)$. The two equations (14) then are solved by $\mathbf{d}_x = -\mathbf{d}_x^{'}$ and $\mathbf{d}_y = -\mathbf{d}_y^{'}$, Fig 5. The force is repulsive and has the magnitude

$$F_{d,hom} = 4\pi K \frac{9d^2}{16h^4}. \tag{16}$$

This force is 1.5 times weaker than $F_{d,planar}$.

IV. CONCLUSION

The nematostatics in 2 and 3 d is very different. The former is very similar to the 2d electrostatics where disclination cores are in place of electric charges. The latter is similar to the electrostatics only in that its Green functions are Coulomb-like. In 3d the counterpart of the electric charge density is a dyad, the elastic charge can be induced only by an external torque whose components play the role of an elastic charge dyad. In this

3d colloidal nematostatics, the Coulomb-like interaction has the reverse sign. We described some implications of the colloidal nematostatics in 3d and showed that, in contrast to the electrostatics, the charges and dipoles are repelled from the wall. One interesting effect is that, applying the field-induced torque on a colloid, one can charge it, Fig.1. If the colloid is an elastic dipole, then by applying the external field one can switch the repulsion from the nematic surface from $1/h^4$ to $1/h^2$ regime. Our results prompt the experimental tests of the interaction in nematic emulsions that, rather than dealing with a pair of particles, can deal with a single colloid at a wall.

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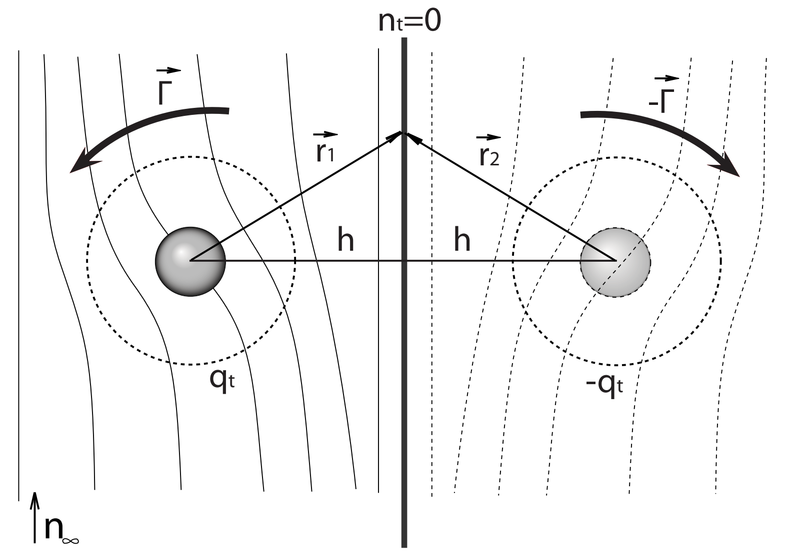

FIG. 2: Elastic charge at a wall with fixed planar director alignment. Elastic charge q_t induced by an external torque $\mathbf{\Gamma}$ and its image $-q_t$ induced by the image-torque $-\mathbf{\Gamma}$. The director at the wall remains unperturbed and equal to $\mathbf{n}_\infty$.

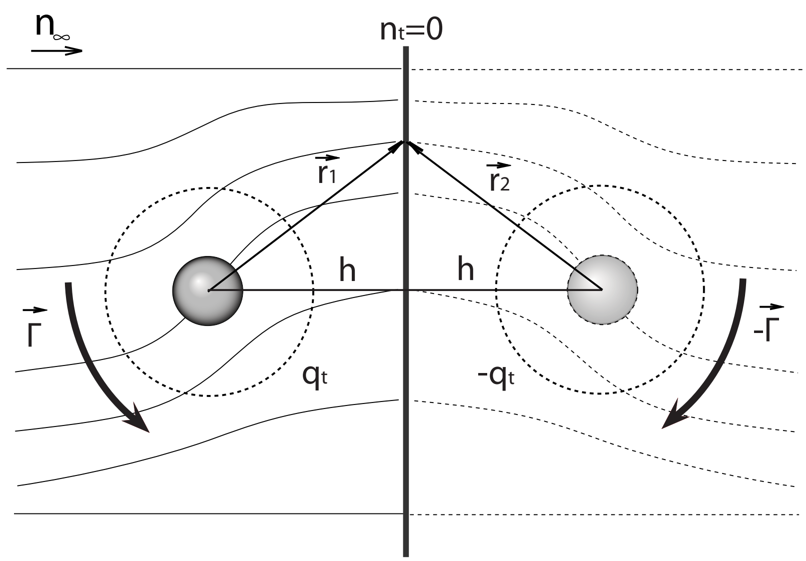

FIG. 3: Elastic charge at a wall with fixed homeotropic director alignment. Elastic charge q_t induced by an external torque $\mathbf{\Gamma}$ and its image $-q_t$ induced by the image-torque $-\mathbf{\Gamma}$. The director at the wall remains unperturbed and equal to $\mathbf{n}_\infty$.

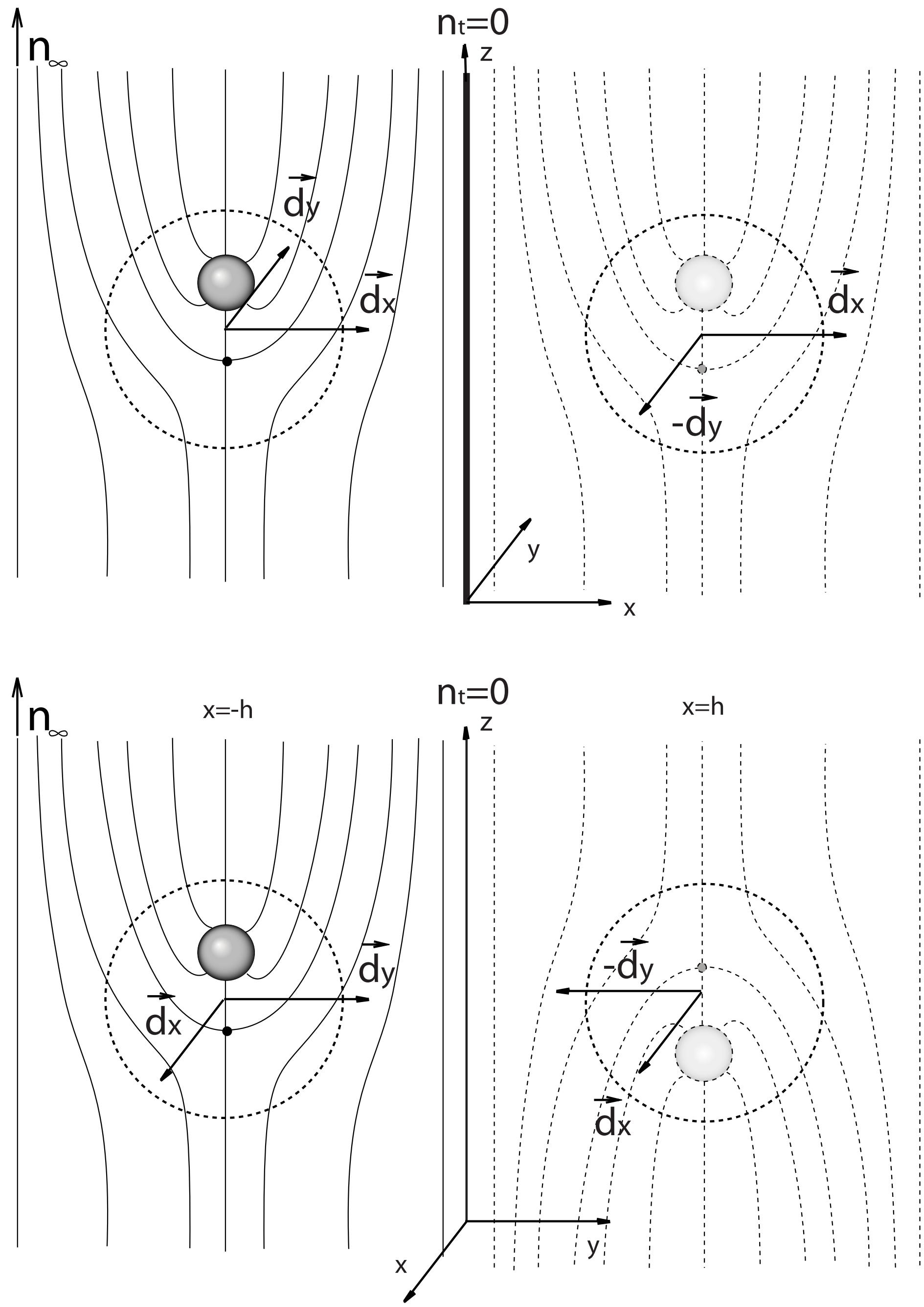

FIG. 4: Dyad of elastic dipole at a wall with fixed planar director alignment. The dipole (left) with $\mathbf{d}_x = (d, 0, 0)$ and $\mathbf{d}_y = (0, d, 0)$ and the image (right) with $\mathbf{d}'_x = (d, 0, 0)$ and $\mathbf{d}'_y = (0, -d, 0)$ shown in two mutually perpendicular planes: a) xz-plane normal to the wall and b) planes $x = -h$ (left) and $x = h$ (right) parallel to the wall.

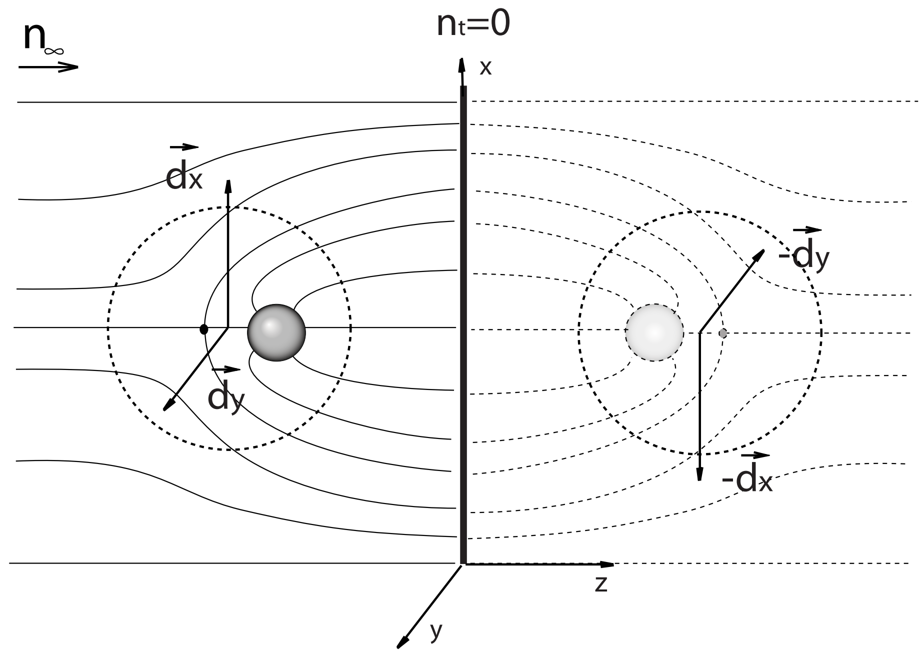

FIG. 5: Dyad of elastic dipole at a wall with fixed homeotropic director alignment. The dipole (left) with $\mathbf{d}_x = (d, 0, 0)$ and $\mathbf{d}_y = (0, d, 0)$ and the image (right) with $\mathbf{d}'_x = (-d, 0, 0)$ and $\mathbf{d}'_y = (0, -d, 0)$ shown in the xz-plane normal to the wall.